

# ADAPTIVE QUADRATURE BY EXPANSION FOR LAYER POTENTIAL EVALUATION IN TWO DIMENSIONS \*

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**Abstract.** When solving partial differential equations using boundary integral equation methods, accurate evaluation of singular and nearly singular integrals in layer potentials is crucial. A recent scheme for this is quadrature by expansion (QBX), which solves the problem by locally approximating the potential using a local expansion centered at some distance from the source boundary. In this paper we introduce an extension of the QBX scheme in 2D denoted AQBX – adaptive quadrature by expansion — which combines QBX with an algorithm for automated selection of parameters, based on a target error tolerance. A key component in this algorithm is the ability to accurately estimate the numerical errors in the coefficients of the expansion. Combining previous results for flat panels with a procedure for taking the panel shape into account, we derive such error estimates for arbitrarily shaped boundaries in 2D that are discretized using panel-based Gauss-Legendre quadrature. Evaluating our scheme on the Laplace and Helmholtz equations we find that the scheme is able to satisfy a given target tolerance to within an order of magnitude, making it useful for practical applications. This represents a significant simplification over the original QBX algorithm, in which choosing a good set of parameters can be hard.

**Key words.** Boundary integral equation, Adaptive, Quadrature, Nearly singular, Error estimate

**AMS subject classifications.** 65R20, 65D30, 65D32, 65G99

**1. Introduction.** Integral equation methods is a class of numerical methods that are based on the reformulation of an elliptic partial differential equation (PDE) as a boundary integral equation. When applicable, this solution approach has several attractive features. Among these are: high-order discretization methods, well-conditioned linear systems after discretization, reduced number of unknowns compared to volume methods, and straightforward handling of moving boundaries.

A suitable starting point for our discussion on integral equation methods is the representation of the solution  $u$  using layer potentials, which are evaluated by integrating the PDE's fundamental solution  $G$  and a layer density  $\sigma$  over the domain boundary  $\partial\Omega$ . By representing  $u$  as a linear combination of the double layer potential  $D$  and the single layer potential  $S$ ,

$$(1) \quad u(z) = D\sigma(z) + \alpha S\sigma(z) = \int_{\partial\Omega} \frac{\partial G(z, w)}{\partial n_w} \sigma(w) ds_w + \alpha \int_{\partial\Omega} G(z, w) \sigma(w) ds_w, \quad z \in \Omega,$$

we get, by considering the limit  $z \rightarrow \partial\Omega$ , a second kind integral equation in  $\sigma$ ,

$$(2) \quad \left( \frac{1}{2}I + D + \alpha S \right) \sigma(z) = f(z), \quad z \in \partial\Omega.$$

This is a generic form of the equations, and we will later define the forms for the interior Laplace and the exterior Helmholtz equations. Here  $f$  is determined by the boundary conditions, and the constant  $\alpha$  is selected such that the integral equation has a unique solution and is well-conditioned [6]. Nyström discretization of this equation using a suitable quadrature rule generates a dense linear system that can be solved rapidly by exploiting the fact that the off-diagonal blocks are of low rank. Solution methods include the fast multipole method (FMM) [10] and fast direct methods [9, 15, 17].

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The main difficulty in the procedure outlined above lies in finding a quadrature rule that can evaluate the layer potentials  $S\sigma(z)$  and  $D\sigma(z)$  when the target point  $z$  is close to or on the boundary  $\partial\Omega$ . Then the integrals of the layer potentials are nearly singular or singular, requiring specialized quadrature methods. For two-dimensional (2D) problems efficient such methods are available, see the summaries [11] and [12]. Some of the methods for two dimensions can be extended to axisymmetric surfaces in three dimensions (3D) [13], but when it comes to general surfaces in 3D the methods are not as mature as in 2D. We refer to [21] for a recent summary of the current state of the art.

**1.1. QBX.** We will in this paper focus on the relatively recent method of quadrature by expansion (QBX) [5, 16]. The method provides a way of evaluating both singular and nearly singular integrals, by representing the layer potential as a local expansion, centered at a point some distance  $r$  away from the boundary. While originally proposed for Helmholtz in 2D, it can be generalized to other PDEs and to 3D, and it has been successfully used in several applications [1, 3, 22]. A strength of QBX is that it uses the same type of local expansions as the FMM, which allows the two methods to be combined into a fast method for evaluating layer potentials at arbitrary locations. This is a topic of ongoing research [20]. As with most methods, however, QBX solves one problem and introduces another. Here the problem solved is that of evaluating layer potentials on or very close to the boundary, and the new problem is how to efficiently compute the local expansion of the layer potential. In particular, computing the expansion coefficients entails evaluating a series of integrals with increasing order of near singularity, so one has effectively traded one hard problem for several easier problems. Nevertheless, QBX is still a competitive method for these problems, especially since it has a solid analytical groundwork [7].

One of the difficulties of QBX is that of parameter selection. The convergence of the local expansion is governed by the order  $p$  at which it is truncated, and by the distance  $r$  between the boundary and the expansion center. The expansion coefficients are computed using a quadrature rule for smooth integrands, and for them to be accurate it is necessary to upsample the boundary points by some factor  $\kappa$ . These three parameters together affect the two competing errors of QBX: the truncation error and the coefficient error (often referred to as the quadrature error). The truncation error increases with  $r$  and decreases with  $p$ , while the coefficient error increases with  $p$  and decreases with  $\kappa$  and  $r$  (see [1, Fig. 3] for an example). Together  $r$ ,  $p$  and  $\kappa$  form a large parameter space, and how to best set these parameters is not clear. Instead, experimentation must be used to determine good parameter ranges for a specific application. This is in itself not unfeasible, but it would be preferable to reduce the number of free parameters.

**1.2. Contribution.** In this paper we propose a scheme for adaptively setting the order  $p$  and upsampling  $\kappa$  at the time of computation, such that the error is maintained below a target tolerance. The key ingredient for this to be successful is the ability to accurately estimate the magnitude of the coefficient error, which is the quadrature error in the expansion coefficients. Such estimates were derived in [2] for simple geometries in two dimensions: flat Gauss-Legendre panels and the trapezoidal rule on the unit circle. Here we extend these estimates, by locally using a polynomial to represent the mapping between a flat panel and a panel of general shape. This greatly increases the accuracy of the estimates, and allows us to build an adaptive QBX scheme based on them. We here restrict ourselves to analyzing Gauss-Legendre panel quadrature, but the methodology could equally well be applied to e.g. a discretization using the trapezoidal rule.

Taking the mapping of the parametrization into account when analyzing nearly singular quadrature errors is by itself not new, a discussion on nearly singular quadrature errors similar to ours can

be found in [5]. Our main contribution in this regard is the construction of an explicit representation of the mapping, which we then invert in order to compute an error estimate.

This paper is organized as follows: In section 2 we introduce the general structure of our scheme, and derive the details for the Laplace double layer potential and the Helmholtz combined field potential. In section 3 we show how to compute the coefficient error estimates necessary for the scheme to be useful. In section 4 we briefly discuss how to combine the scheme with a fast method. In section 5 we show a selection of numerical results to illustrate the performance of our method.

**2. Foundations of AQBX.** In this section we begin by introducing the foundations of our method using a generic notation, before we give the specific details for the Laplace and Helmholtz equations. We start from a given layer potential representation,

$$(3) \quad u(z) = \int_{\partial\Omega} G(z, w) \sigma(w) \, ds_w.$$

To evaluate this using AQBX, we first need to split the fundamental solution using a suitable addition theorem,

$$(4) \quad G(z, w) = \sum_{m=0}^{\infty} A_m^r(w, z_0) \cdot B_m^r(z, z_0),$$

which for a given  $r$  is valid for

$$(5) \quad |z - z_0| < r \leq |w - z_0|.$$

For the specific formulas for Laplace and Helmholtz, see (25) and (36). We assume that (4) is normalized such that the following holds:

$$(6) \quad |B_m^r(z - z_0)| = \begin{cases} \leq 1, & |z - z_0| \leq r, \\ \mathcal{O}(1), & |z - z_0| = r. \end{cases}$$

By the last condition we mean that although the only strict requirement on  $|B_m^r|$  is that it is bounded by 1, we prefer it to be close to 1 at  $|z - z_0| = r$ . The addition theorem allows us to pick an expansion center  $z_0$ , determine  $r$  as

$$(7) \quad r = \min_{w \in \partial\Omega} |w - z_0|,$$

and evaluate the layer potential as a local expansion in the neighborhood of  $z_0$ ,

$$(8) \quad u(z) = \sum_{m=0}^{\infty} a_m \cdot B_m^r(z, z_0), \quad |z - z_0| \leq r,$$

where

$$(9) \quad a_m = \int_{\partial\Omega} A_m^r(w, z_0) \sigma(w) \, ds_w.$$

The fact that (8) holds also at the equality  $|z - z_0| = r$  was shown in [7] for the Laplace and Helmholtz equations, but can be generalized to other kernels, e.g. Stokes equations [1]. This is what allows us to evaluate the expansion also on  $\partial\Omega$ , at the single point which is closest to  $z_0$ .

In a computational scheme the local expansion is truncated at a maximum order  $p$ , and the coefficients, which we now denote  $\tilde{a}_m$ , are computed using a suitable quadrature rule. This gives us the QBX approximation of the layer potential,

$$(10) \quad u_p(z) = \sum_{m=0}^p \tilde{a}_m \cdot B_m^r(z, z_0).$$

The error in this approximation can be separated into a truncation error  $e_T$  and a coefficient error  $e_C$  [7],

$$(11) \quad u(z) - u_p(z) = \underbrace{u(z) - \sum_{m=0}^p a_m \cdot B_m^r(z, z_0)}_{e_T} + \underbrace{\sum_{m=0}^p (a_m - \tilde{a}_m) \cdot B_m^r(z, z_0)}_{e_C}.$$

**2.1. Truncation error.** The truncation error  $e_T$  of the scheme arises because we limit the local expansion to  $p + 1$  terms. In our normalized form (6) it can be bounded by

$$(12) \quad |e_T| = \left| \sum_{m=p+1}^{\infty} a_m \cdot B_m^r(z, z_0) \right| \leq \sum_{m=p+1}^{\infty} |a_m|.$$

It was shown in [7] that the truncation error for several kernels behaves like

$$(13) \quad e_T \leq M(p, r) r^{p+1} \|u\|_{C^{p+1}(|z-z_0| \leq r)}.$$

One can in practice observe that the error decays exponentially in  $p$  with a rate that is proportional to  $r$ ,

$$(14) \quad e_T \sim (cr)^p,$$

where  $c$  is a constant that depends on the local regularity of  $u$ . Finding an a priori estimate for  $c$  is hard, since it depends on both the local geometry of  $\partial\Omega$  and the regularity of the density  $\sigma$  in a nontrivial way. However, since the terms of the local expansion decay exponentially, a good estimate for the truncation error is

$$(15) \quad |e_T| \approx \left| a_{p+1} \cdot B_{p+1}^r(z, z_0) \right| \leq |a_{p+1}|.$$

In practice we only have the coefficients up to  $a_p$ . Therefore, we can define a useful (and usually conservative) a posteriori estimate as

$$(16) \quad |e_T| \approx \left| a_p \cdot B_p^r(z, z_0) \right| \leq |a_p|.$$

**2.2. Coefficient error.** The coefficient error  $e_C$  in (11) is a result of the numerical evaluation of the coefficient integrals (9) for  $m = 0, \dots, p$ , which for a given boundary  $\partial\Omega$  is evaluated using some  $n$ -point quadrature rule. Assuming that the density  $\sigma$  and the boundary  $\partial\Omega$  are well-resolved by that quadrature (which is a prerequisite for the underlying Nyström discretization), the main source of the error is the near singularity in  $A_m^r$  when evaluated at  $z_0$ . The order of this near singularity typically grows with  $m$ , and to counter this the density must be upsampled (by interpolation) to a grid which is fine enough to resolve  $A_m^r$ . The amount of upsampling required can be determined through  $E_C(n, m)$ , which is an accurate a priori estimate of the coefficient error in term  $m$  when using  $n$  quadrature nodes,

$$(17) \quad E_C(n, m) \approx |a_m - \tilde{a}_m| \geq |(a_m - \tilde{a}_m) \cdot B_m^r(z, z_0)|.$$

We will in section 3 show how to derive such error estimates for the cases of the Laplace and Helmholtz equations.

**REMARK 1** (Resolution error). *Here we only discuss errors in the coefficients  $\tilde{a}_m$  due to near singularities in the integrals (9). However, there is also a lower bound on the accuracy of the coefficients, imposed by how well the underlying grid resolves the boundary  $\partial\Omega$  and the layer density  $\sigma$ . For a given panel, this resolution error could be estimated by analyzing a modal expansion of the grid point coordinates and density values, such as the Legendre polynomial expansion used in section 3. Such an analysis is however beyond the scope of the present paper.*

**2.3. The AQBX scheme.** Let us now assume that we have a discretization of  $\partial\Omega$  characterized by  $n$ , which for a global quadrature denotes the total number of points, and for a panel-based quadrature denotes the number of points on each panel. Denoting that quadrature  $Q_n$ , we define a combined interpolation and quadrature operator  $Q_{\kappa n}$ , which computes the quadrature by first upsampling the density to  $\kappa n$  points (for simplicity we assume  $\kappa$  integer). Furthermore, we assume that the error when computing a coefficient  $a_m$  is well estimated by a function  $E_C(\kappa n, m)$ . Then the adaptive algorithm for evaluating  $u(z)$  in the neighborhood of  $z_0$  to a tolerance  $\epsilon$  can be summarized using Algorithms 1 and 2.

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**Algorithm 1** Compute expansion coefficients at  $z_0$  to tolerance  $\epsilon$ .

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```

function EXPANSION_COEFFICIENTS( $z_0, \epsilon$ )
   $\kappa \leftarrow 1, m \leftarrow 0$ 
  repeat
    while  $E_C(\kappa n, m) > \epsilon$  do                                 $\triangleright$  Check  $e_C$  estimate
       $\kappa \leftarrow \kappa + 1$                                            $\triangleright$  Increase upsampling rate
    end while
     $a_m \leftarrow Q_{\kappa n}[A_m^r(\cdot, z_0)\sigma(\cdot)]$                    $\triangleright$  Compute coefficient
     $m \leftarrow m + 1$ 
  until  $|a_m| < \epsilon$                                               $\triangleright$  Break when  $e_T$  estimate below tolerance
  return  $\{a_m\}$ 
end function

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**Algorithm 2** Evaluate  $u(z)$  to tolerance  $\epsilon$  using expansion at  $z_0$ .

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function EVALUATE_EXPANSION( $z, z_0, \{a_m\}, \epsilon$ )
   $u \leftarrow 0, m \leftarrow 0$ 
  repeat
     $\delta_m \leftarrow a_m \cdot B_m^r(z, z_0)$  ▷ Evaluate  $m$ th expansion term
     $u \leftarrow u + \delta_m$ 
     $m \leftarrow m + 1$ 
  until  $|\delta_m| < \epsilon$  ▷ Break when  $e_T$  estimate below tolerance
  return  $u$ 
end function

```

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Note that if Algorithm 1 has produced  $p + 1$  coefficients, then Algorithm 2 is guaranteed to terminate within  $p + 1$  iterations, since  $|\delta_p| \leq |a_p| < \epsilon$ . For more conservative termination criteria, one can use  $\max(|a_{m-1}|, |a_m|) < \epsilon$  and  $\max(|\delta_{m-1}|, |\delta_m|) < \epsilon$  to take into account any even/odd behavior in the expansion.

**2.4. Specific applications.** We will now proceed with formulating AQBX for two different applications: the Laplace double layer potential and the Helmholtz combined field potential.

**2.4.1. Laplace equation.** We first consider the Laplace Dirichlet problem in a domain  $\Omega$  bounded by a boundary  $\partial\Omega$ ,

$$(18) \quad \Delta u = 0, \quad \text{in } \Omega,$$

$$(19) \quad u = g, \quad \text{on } \partial\Omega.$$

The fundamental solution to this PDE is

$$(20) \quad \phi(z, w) = \frac{1}{2\pi} \log|z - w|.$$

The interior Dirichlet problem can be represented using the double layer potential,

$$(21) \quad u(z) = D\sigma(z) = \int_{\partial\Omega} \frac{\partial\phi(z, w)}{\partial n_w} \sigma(w) ds_w,$$

where  $n_w$  denotes the unit normal. In complex notation this can be compactly represented as

$$(22) \quad u(z) = \operatorname{Re} v(z),$$

$$(23) \quad v(z) = \frac{-1}{2\pi} \int_{\partial\Omega} \frac{n_w}{z - w} \sigma(w) ds_w.$$

On  $\partial\Omega$  the density  $\sigma$  satisfies the integral equation

$$(24) \quad \left( \frac{1}{2}I + D \right) \sigma = f.$$

It should be noted that this particular layer potential actually has a smooth limit on the boundary, so no special quadrature is needed for solving the integral equation, unless different parts of the boundary are close to each other. Special quadrature is however still needed for evaluating the solution close to the boundary, once  $\sigma$  has been computed.

Starting from the Taylor expansion of the Cauchy kernel,

$$(25) \quad \frac{-1}{z-w} = \sum_{j=0}^{\infty} \frac{(z-z_0)^j}{(w-z_0)^{j+1}},$$

it is straightforward to derive the AQBX formulation (4) for  $v(z)$ ,

$$(26) \quad A_m^r(w, z_0) = \frac{r^m n_w}{2\pi(w-z_0)^{m+1}},$$

$$(27) \quad B_m^r(z, z_0) = \frac{(z-z_0)^j}{r^m}.$$

Note that, by these definitions together with (9), the real part of the coefficient  $a_0$  will simply hold the value of the double layer potential evaluated at  $z_0$ , i.e.  $\text{Re } a_0 = u(z_0)$ .

**2.4.2. Helmholtz equation.** We now consider the Helmholtz Dirichlet problem in an unbounded domain  $\Omega$  exterior to a boundary  $\partial\Omega$ , which for a wavenumber  $k$  is stated as

$$(28) \quad \Delta u + k^2 u = 0, \quad \text{in } \Omega,$$

$$(29) \quad u = f, \quad \text{on } \partial\Omega.$$

The solution must satisfy the Sommerfeld radiation condition for  $r = |z|$ ,

$$(30) \quad \lim_{r \rightarrow \infty} r^{1/2} \left( \frac{\partial u}{\partial r} - iku \right) = 0.$$

The fundamental solution is essentially the zeroth-order Hankel function of the first kind,

$$(31) \quad \phi_k(z, w) = \frac{i}{4} H_0^{(1)}(k|z-w|).$$

The solution can be represented using the combined field integral representation<sup>1</sup>,

$$(32) \quad u(z) = \int_{\partial\Omega} \left( \frac{\partial \phi_k(z, w)}{\partial n_w} - \frac{ik}{2} \phi_k(z, w) \right) \sigma(w) \, ds_w = \left( D_k \sigma - \frac{ik}{2} S_k \sigma \right) (z).$$

The double layer kernel is

$$(33) \quad \frac{\partial \phi_k(z, w)}{\partial n_w} = \frac{ik}{4} H_1^{(1)}(k|z-w|) \frac{(z-w) \cdot n_w}{|z-w|}$$

$$(34) \quad = \frac{ik}{4} H_1^{(1)}(k|z-w|) |z-w| \, \text{Re} \left[ \frac{n_w}{z-w} \right].$$

On the boundary we get the integral equation

$$(35) \quad \left( \frac{1}{2} I + D_k - \frac{ik}{2} S_k \right) \sigma = f.$$

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<sup>1</sup>The general form of the representation is  $D_k - i\eta S_k$ . We have here set  $\eta = k/2$ , following [12].

To formulate AQBX for the combined field representation, we start from the Graf addition theorem [18, §10.23(ii)],

$$(36) \quad \frac{i}{4} H_0^{(1)}(k|z-w|) = \sum_{m=-\infty}^{\infty} \frac{i}{4} H_m^{(1)}(kr_w) e^{-im\theta_w} J_m(kr_z) e^{im\theta_z}, \quad r_z < r_w.$$

Here  $(r_w, \theta_w)$  and  $(r_z, \theta_z)$  are the polar coordinates of  $w - z_0$  and  $z - z_0$ ,

$$(37) \quad \begin{aligned} r_w &= |w - z_0|, & r_z &= |z - z_0|, \\ e^{-im\theta_w} &= \frac{|w - z_0|^m}{(w - z_0)^m}, & e^{im\theta_z} &= \frac{(z - z_0)^m}{|z - z_0|^m}. \end{aligned}$$

The Bessel functions  $J_m$  decay rapidly with  $m$ . It is however easy to experimentally verify that a normalization satisfying (6) is obtained by using the first term of the power series for  $J_m(kr)$  [18, §10.4, §10.8],

$$(38) \quad J_{\pm m}(kr) = (\pm 1)^m \frac{1}{m!} \left(\frac{kr}{2}\right)^m + \mathcal{O}\left(\frac{1}{(m+1)!} \left(\frac{kr}{2}\right)^{m+2}\right), \quad m \geq 0.$$

This gives us the AQBX formulation (4) for the combined field representation,

$$(39) \quad A_0^r(w, z_0) = \left(d_0(w, z_0) - \frac{ik}{2} s_0(w, z_0), 0\right),$$

$$(40) \quad B_0^r(z, z_0) = (J_0(kr_z), 0).$$

and, for  $m > 0$ ,

$$(41) \quad A_m^r(w, z_0) = \frac{\sqrt{2}}{m!} \left(\frac{kr}{2}\right)^m \left(d_m(w, z_0) - \frac{ik}{2} s_m(w, z_0), d_{-m}(w, z_0) - \frac{ik}{2} s_{-m}(w, z_0)\right),$$

$$(42) \quad B_m^r(z, z_0) = \frac{m!}{\sqrt{2}} \left(\frac{2}{kr}\right)^m \left(J_m(kr_z) e^{im\theta_z}, J_{-m}(kr_z) e^{-im\theta_z}\right).$$

Here  $s_m$  is an immediate result of (36),

$$(43) \quad s_m(w, z_0) = \frac{i}{4} H_m^{(1)}(kr_w) e^{-im\theta_w},$$

while  $d_m$  is obtained by differentiation of (43). A compact form for  $d_m$  was derived in [5],

$$(44) \quad d_m(w, z_0) = \frac{ik}{8} \left(H_{m-1}^{(1)}(kr_w) e^{-i(m-1)\theta_w} \bar{n}_w - H_{m+1}^{(1)}(kr_w) e^{-i(m+1)\theta_w} n_w\right).$$

We again note that the coefficient  $a_0$  (9) will hold the value of the potential at  $z_0$ , since (trivially)  $s_0 = \phi_k$  in (31) and (through (34))

$$(45) \quad d_0(w, z_0) = -\frac{ik}{4} H_1^{(1)}(kr_w) \operatorname{Re} \left[e^{-i\theta_w} n_w\right] = \frac{\partial \phi_k(z_0, w)}{\partial n_w}.$$



**3. Coefficient errors.** In this section we derive a central piece of AQBx: the coefficient error estimate  $E_C$  required in Algorithm 1. We will consider the layer potentials of section 2.4 combined with a panel-based quadrature, where the boundary curve subdivided into smaller segments, each of which is discretized using an  $n$ -point Gauss-Legendre quadrature. This is sometimes referred to as a composite Gauss-Legendre quadrature.

We begin by considering the error in the contribution to a coefficient from a single panel; the total error can then be computed as the sum of errors from all adjacent panels. For this, let  $\Gamma$  be an open curve (i.e. a panel) parametrized by an analytic function  $\gamma(t) \in \mathbb{C}$ ,  $t \in [-1, 1]$ , with the normal defined as  $n(t) = i\gamma'(t)/|\gamma'(t)|$ . For simplicity we denote by  $\sigma(t)$  the pullback of  $\sigma$  under  $\gamma$ , i.e.  $\sigma(t) = \sigma(\gamma(t))$ .

**3.1. Laplace coefficient error.** Beginning with QBx for the Laplace double layer potential (sec. 2.4.1), the expansion coefficients are computed as

$$(46) \quad a_m = \frac{r^m}{2\pi} \int_{\Gamma} \frac{\sigma(w)n_w}{(w - z_0)^{m+1}} ds_w$$

$$(47) \quad = \frac{ir^m}{2\pi} \int_{-1}^1 \frac{\sigma(t)}{(\gamma(t) - z_0)^{m+1}} \gamma'(t) dt.$$

The coefficient errors are introduced when this integral is evaluated using a discrete quadrature rule. In a boundary integral equation context, we assume a panel  $\Gamma$  such that  $\gamma$  and  $\sigma$  are well-resolved by an  $n$ -point Gauss-Legendre quadrature rule. We will here focus on the standard choice  $n = 16$ . Denoting by  $I$  the integral over  $[-1, 1]$ , and by  $Q_n$  the Gauss-Legendre approximation of that integral, the quadrature error is defined as

$$(48) \quad R_n = I - Q_n.$$

If the above assumptions on the resolution hold, then we can expect the quadrature error to be small for the integrand (47), provided that  $z_0$  is far away from  $\Gamma$ . If on the other hand  $z_0$  is close to  $\Gamma$ , then the quadrature error will be dominated by the nearly singular quadrature error that arises when the integrand is evaluated close to its pole.

To estimate nearly singular quadrature errors, we can use the results and methods of [2], which rely on contour integration and calculus of residues for deriving accurate estimates. The main result which we want to use is the following:

**LEMMA 1** (Adapted from [2]). *Let  $f(t)$  be a meromorphic function which is analytic on  $[-1, 1]$  and has pole  $t_0 \in \mathbb{C}$  of order  $m + 1$  lying close to that interval. If  $f$  is integrated on  $[-1, 1]$  using the  $n$ -point Gauss-Legendre rule, then the quadrature error (48) is well approximated by*

$$(49) \quad R_n[f] \approx -\text{Res}[f(t)k_n(t), t_0] = -\frac{1}{m!} \lim_{t \rightarrow t_0} \frac{d^m}{dt^m} \left( (t - t_0)^{m+1} f(t) k_n(t) \right),$$

where  $k_n$  is the characteristic remainder function, and can be approximated as

$$(50) \quad k_n(t) \approx \frac{2\pi}{(t + \sqrt{t^2 - 1})^{2n+1}}.$$

Moreover, if  $f(t)k_n(t) \rightarrow 0$  as  $|t| \rightarrow \infty$ , then the error in the approximation (49) goes to zero in the limit  $n \rightarrow \infty$ .

REMARK 2. When evaluating  $k_n(t)$  numerically, care must be taken with respect to the branch cut of the square root. The function is however doubly symmetric in the  $t$ -plane, so a safe way of evaluating it is to first transform  $t$  to the first quadrant, i.e.  $k_n(t) \rightarrow k_n(t^*)$ , where  $t^* = |\operatorname{Re} t| + i|\operatorname{Im} t|$ .

The integral (46) clearly has a pole of order  $m + 1$  at  $z_0$ . In parametrized form (47) the pole instead lies at the point  $t_0 \in \mathbb{C}$ , such that

$$(51) \quad \gamma(t_0) - z_0 = 0.$$

Note that evaluating  $\gamma(t_0)$  corresponds to evaluating an analytic continuation of  $\gamma(t)$  in some neighborhood of  $[-1, 1]$ . Denoting by  $\tilde{a}_m$  the approximation of  $a_m$  (as defined in (47)), and also assuming that there exists an analytic continuation of  $\sigma$ , then we have from Lemma 1 that

$$(52) \quad a_m - \tilde{a}_m = R_n \left[ \frac{ir^m \sigma \gamma'}{2\pi(\gamma - z_0)^{m+1}} \right] \approx -\frac{ir^m}{2\pi m!} \lim_{t \rightarrow t_0} \frac{d^m}{dt^m} \left( (t - t_0)^{m+1} \frac{\sigma(t) \gamma'(t)}{(\gamma(t) - z_0)^{m+1}} k_n(t) \right).$$

To simplify this we first assume that  $k_n$  varies much more rapidly than the other factors in the differentiation, such that a good approximation is obtained by only considering the term with the  $m$ th derivative of  $k_n$ . This can be motivated by our assumptions on resolution. Second, we note that since  $z_0 = \gamma(t_0)$ ,

$$(53) \quad \lim_{t \rightarrow t_0} \frac{(t - t_0)^{m+1}}{(\gamma(t) - z_0)^{m+1}} = \frac{1}{(\gamma'(t_0))^{m+1}}.$$

Thus a coefficient error estimate  $E_C(n, m) \approx |a_m - \tilde{a}_m|$  is given by

$$(54) \quad E_C(n, m) = \frac{r^m |\sigma(t_0)|}{2\pi m! |\gamma'(t_0)|^m} |k_n^{(m)}(t_0)|.$$

The derivatives of  $k_n$  can (at least for small  $m$ ) be derived analytically from (50), or, as shown in [2], approximated as

$$(55) \quad k_n^{(m)}(t) \approx k_n(t) \left( -\frac{2n+1}{\sqrt{t^2-1}} \right)^m.$$

The estimate (54) using (55) holds well in the limit  $n \rightarrow \infty$ , but will lose accuracy with increasing  $m$  for a fixed  $n$ . We have in practice found that it starts losing its reliability around  $m > n/2$ , so that it then is safer to trigger an upsampling in Algorithm 1, instead of continuing to rely on the estimate.

Though the above derivation is rather straightforward, some more work is required if we want to evaluate (54) in practice, since that requires finding  $t_0$  and being able to evaluate  $\sigma(t_0)$  and  $\gamma(t_0)$ . For this, one would ideally like to have access to analytic expressions for  $\sigma$  and  $\gamma$ , but what we typically have is instead the values of the functions at the quadrature nodes. To be able to evaluate (54) using this pointwise data, we first need to construct continuations of  $\gamma$  and  $\sigma$ . Then we need to solve (51) using the continuation of  $\gamma$ , in order to find  $t_0$  and finally evaluate the estimate. This may sound hard, but can actually be done in a stable and efficient way using polynomial extrapolation.

Beginning with the continuation of  $\gamma$ , let  $t_i$  and  $w_i$ ,  $i = 1 \dots n$ , be the nodes and weights of the  $n$ -point Gauss-Legendre quadrature. We can then let  $P_n[\gamma](t)$  be the polynomial of degree

$n - 1$  that interpolates  $\gamma(t)$  at the nodes  $t_i$ . The distribution of  $t_i$  ensures that we can form such a high-degree polynomial ( $n = 16$ ) without being troubled by the ill-conditioning known as Runge's phenomenon. We use as our basis the Legendre polynomials  $P_\ell(t)$ ,

$$(56) \quad P_n[\gamma](t) = \sum_{\ell=0}^{n-1} \hat{\gamma}_\ell P_\ell(t),$$

which through their orthogonality allow us to compute the coefficients  $\hat{\gamma}_\ell$  in an efficient and well-conditioned way,

$$(57) \quad \hat{\gamma}_\ell = \frac{2\ell+1}{2} \sum_{i=1}^n P_\ell(t_i) w_i \gamma(t_i), \quad \ell = 0, \dots, n-1.$$

To further improve conditioning in our method, we assume that  $\Gamma$  has endpoints at  $-1$  and  $1$ ; this can be achieved for any open curve by first applying a simple scaling and rotation to both  $\Gamma$  and  $z_0$ . Letting the interpolant  $P_n[\gamma](t)$  be the analytic continuation of  $\gamma(t)$ , we can now find  $t_0$  in (51) by instead solving

$$(58) \quad P_n[\gamma](t_0) = z_0.$$

This does, for the purposes of error estimation, work very well in the near neighborhood of  $\Gamma$ , see example in Figure 1. Equation (58) can be solved efficiently using Newton's method, but the choice of starting guess can be important, especially near concave regions of the curve (e.g. below the curve of Figure 1). In such regions the inverse mapping  $t_0 = \gamma^{-1}(z_0)$  is no longer single-valued, and for our estimate to be accurate we want the solution  $t_0$  that predicts the largest error, when the estimate is evaluated at that point. This "worst solution" can often be found by solving with  $t_0 = \pm 1$  as starting guesses and comparing the results; this strategy was used for the results shown to the right in Figure 2. As an alternative, one can use  $t_0 = z_0$  as starting guess (given the above assumptions on the endpoints of  $\Gamma$ ). This simpler strategy works well for practical purposes, and is what we use throughout the remainder of this paper.

Once  $t_0$  is found, we are able to evaluate the coefficient error estimate as given in (54). The value of  $\gamma'(t_0)$  can be found by differentiation of the interpolant,

$$(59) \quad \gamma'(t_0) = P'_n[\gamma](t_0).$$

We can also evaluate  $\sigma(t_0)$  through an interpolating polynomial,

$$(60) \quad \sigma(t_0) = P_n[\sigma](t_0).$$

This works very well if  $\sigma$  is well-resolved on  $\Gamma$ , and can be used to obtain the fine-scale correspondence between error and estimate seen in Figure 3. A less expensive alternative is to use the max norm of  $\sigma$  on the interval/panel,

$$(61) \quad \sigma(t_0) \approx \|\sigma(t)\|_{L^\infty(-1,1)} = \|\sigma(z)\|_{L^\infty(\Gamma)}.$$

This works well in practice, and also appears to be slightly more robust whenever  $\sigma$  is not fully resolved on  $\Gamma$ , especially for Helmholtz. We use this approach in the results of section 5.

The above results can also be used for estimating the nearly singular quadrature error when evaluating the double layer potential (21) near  $\Gamma$ , and hence to determine when AQBX needs to

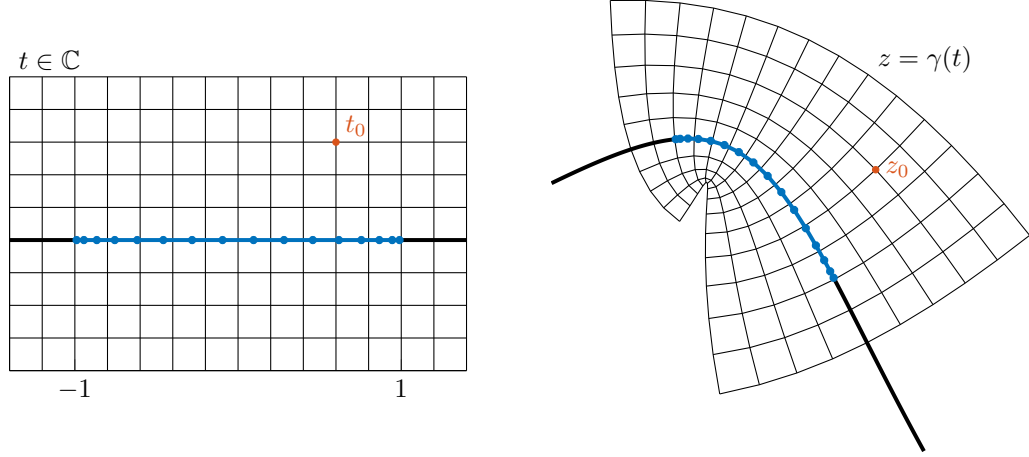


FIG. 1. Illustration of how the analytic continuation of  $\gamma$  maps the vicinity of  $[-1, 1]$  to the space surrounding  $\Gamma$ . Here  $\Gamma$  is a segment of the starfish domain seen in Figure 3. Polynomial interpolation of  $\gamma$  on a 16-point panel gives a locally very accurate approximation of the continuation:  $|\gamma - P_n[\gamma]| < 10^{-7}$  on the shown grid.

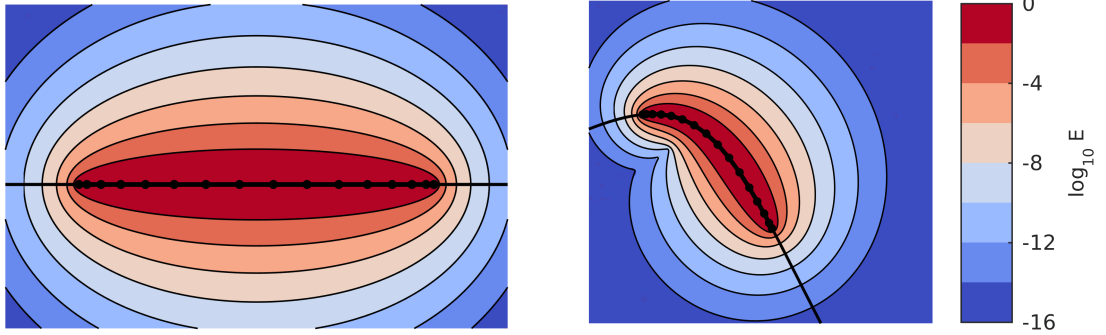


FIG. 2. Quadrature errors when evaluating the integral (47) for  $m = 0$  and  $\sigma = 1$  on a flat and a curved panel. These panels correspond to those shown in Figure 1. Colored fields are actual error levels, contour lines are computed using the error estimate (54) with  $t_0$  determined by inverting  $P_n[\gamma](t)$ . The ellipses to the left have foci in  $\pm 1$ , and are also known as Bernstein ellipses.

be used. To that end, we simply use the observation that  $u(z_0) = \text{Re } a_0$ . Denoting by  $\tilde{u}(x)$  the potential evaluated using direct quadrature, we thus have from (52) that

$$(62) \quad |u(z) - \tilde{u}(x)| \approx \frac{1}{2\pi} \left| \text{Im} [\sigma(t_0) k_n(t_0)] \right|.$$

This estimate, when evaluated using the above procedure, is very accurate. As an example, in Figure 3, we consider the Laplace Dirichlet problem in a starfish domain. The density is computed by solving (24) using the Nyström method and a right-hand side given by a collection of point sources (marked by + in the figure). The solution is then evaluated inside the domain directly using the composite Gauss-Legendre quadrature, and compared to the reference solution given by the boundary condition. Comparing these results to those in [2, fig. 7], which used a flat panel

approximation, shows the importance of taking into the account the inverse mapping of the target point.

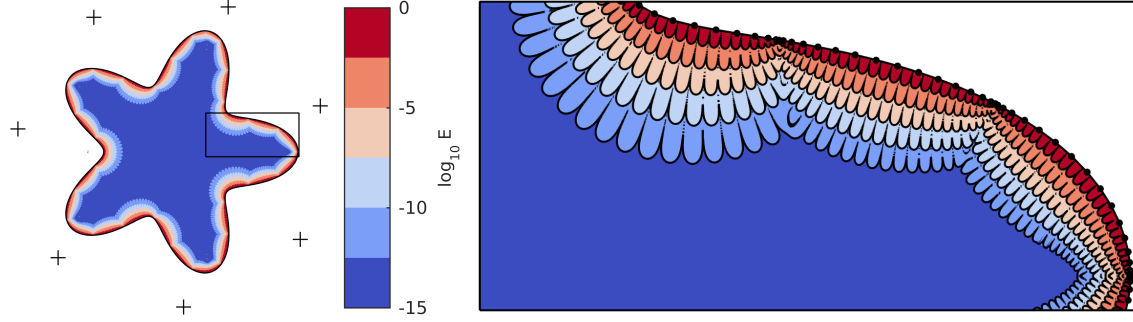


FIG. 3. Error curves when evaluating the Laplace double layer potential directly using 27 panels of equal arc length, with 16 points on each panel. Colored fields represent the error compared to the exact solution, contour lines are computed using the estimate (62) with (60), and coincide almost perfectly with the actual error.

**3.2. Helmholtz coefficient error.** We now turn to AQBx for the Helmholtz combined field potential (sec. 2.4.2). When evaluating the expansion coefficients, the Hankel functions in the integrands have a singularity as  $r_w \rightarrow 0$ , which to leading order behaves like [18, §10.4, §10.8]

$$(63) \quad H_{\pm l}^{(1)}(kr_w) = -(\pm 1)^l \frac{2^l (l-1)!}{\pi} (kr_w)^{-l} + \mathcal{O}\left((kr_w)^{-(l-2)}\right).$$

The quadrature error due to near singularity is dominated by that from the highest-order pole, so for the purposes of error estimation it is suitable to only keep the highest-order Hankel function in the expression for (41), and to approximate that Hankel function using only the first term of (63). We can then approximate (43) as

$$(64) \quad s_m(w, z_0) \approx 0,$$

and (44) as

$$(65) \quad d_0(w, z_0) = -\frac{ik}{4} H_1^{(1)}(kr_w) r_w \operatorname{Re} \left[ \frac{n_w}{w - z_0} \right]$$

$$(66) \quad \approx \frac{1}{2\pi} \operatorname{Re} \left[ \frac{n_w}{w - z_0} \right],$$

and, for  $|m| > 0$  and using (37),

$$(67) \quad d_m(w, z_0) \approx \frac{k}{8} H_{|m|+1}^{(1)}(kr_w) e^{-i(|m|+1)\theta_w} n_w$$

$$(68) \quad \approx \frac{k}{8\pi} 2^{|m|+1} |m|! (kr_w)^{-(|m|+1)} e^{-i(|m|+1)\theta_w} n_w$$

$$(69) \quad = \frac{2^{|m|} |m|!}{4\pi k^{|m|}} \frac{n_w}{(w - z_0)^{|m|+1}}.$$

Inserted into (41), this gives

$$(70) \quad A_0^r(w, z_0) \approx (1, 0) \frac{1}{2\pi} \operatorname{Re} \left[ \frac{n_w}{w - z_0} \right],$$

$$(71) \quad A_m^r(w, z_0) \approx \sqrt{2} (1, 1) \frac{r^m}{4\pi} \frac{n_w}{(w - z_0)^{m+1}}, \quad m > 0.$$

Note that we in the above series of simplifications have removed constant factors which are irrelevant to the magnitude of the error (i.e.  $-1$  and  $i$ ). Estimating the error of these simplified integrands on a panel with parametrization  $\gamma$ , it follows that

$$(72) \quad |a_0 - \tilde{a}_0| \approx \left| \operatorname{Im} R_n \left[ \frac{\sigma \gamma'}{2\pi(\gamma - z_0)} \right] \right|,$$

$$(73) \quad |a_m - \tilde{a}_m| \approx \left| R_n \left[ \frac{r^m \sigma \gamma'}{2\pi(\gamma - z_0)^{m+1}} \right] \right|, \quad m > 0.$$

Note that (72) is bounded by (73) with  $m = 0$ , so it is sufficient to use only (73), if we can accept being on the conservative side for  $m = 0$ . Also note that the integrand in (73) is exactly the same as in the error estimate for the Laplace double layer potential (52). The conclusion is that, remarkably, the coefficient error estimate  $E_C$  for Helmholtz is identical to that previously derived for Laplace (54),

$$(74) \quad E_C(n, m) = \frac{r^m |\sigma(t_0)|}{2\pi m! |\gamma'(t_0)|^m} |k_n^{(m)}(t_0)|.$$

This correspondence between Laplace and Helmholtz also holds for the quadrature error when evaluating the underlying potential itself. This can be seen from (72) and the observation from (45) that  $a_0 = (u(z_0), 0)$ ,

$$(75) \quad |u(x) - \tilde{u}(x)| \approx \frac{1}{2\pi} \left| \operatorname{Im} [\sigma(t_0) k_n(t_0)] \right|$$

$$(76) \quad \leq \frac{1}{2\pi} |\sigma(t_0) k_n(t_0)|.$$

This estimate has been derived by simplifying the Helmholtz double layer kernel and noting that the leading singularity is identical to that of the Laplace double layer. However, in experiments we can observe that the small-scale oscillations predicted by (75) (and which are clearly noticeable in the Laplace case) only appear for small wavenumbers, and it is therefore generally better to use (76). As a demonstration, in Figure 4 we repeat the experiment of Figure 3, but for the Helmholtz exterior Dirichlet problem. We set a number of point sources (marked  $+$ ) inside a starfish domain and solve the integral equation (35) using the discretization scheme of [12]. The correspondence between error and estimate is still very good, though not as excellent as in the Laplace case.

It is worth noting that the error estimate (76) is independent of the wavenumber  $k$ . This might come as a surprise, as one usually needs to increase the grid resolution with increasing wavenumber. However, here we only take into account the nearly singular quadrature error, under the assumption that far-field interactions are well-resolved. The result simply reflects the fact that the singularity in the kernel is independent of  $k$ .

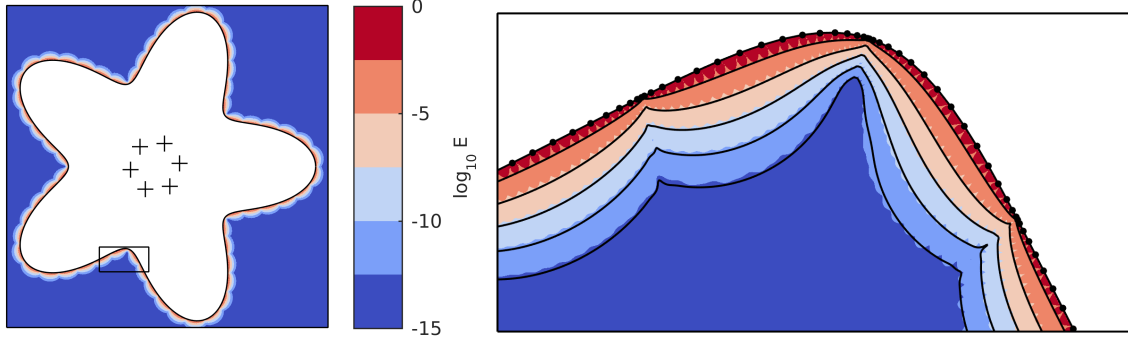


FIG. 4. Error curves when evaluating the Helmholtz combined field potential directly using 60 panels of equal arc length, with 16 points on each panel. The wavenumber is set to  $k = 4/h$ ,  $h$  being the length of the panels. Colored fields represent the error compared to the exact solution, contour lines are computed using the estimate (76) with (60).

**4. Local AQBX.** Since QBX is a special quadrature scheme for target points that are close to or on the boundary  $\partial\Omega$ , it makes sense to only use QBX for those parts of the boundary that are close to a given target point. This is known as “local QBX” [19] (as opposed to “global QBX”), and can be particularly straightforward to combine with a fast method. For panel-based quadrature on a simple curve this is easy to implement; only the panels that are near a given expansion center are used in the local expansion. Selecting panels to include can be done using an error estimate of the layer potential, such as (62) in combination with a tolerance, or by simply including a fixed number of neighboring panels (this works well if all panels are of equal length). When evaluating the potential, the contribution from the near panels is computed through the local expansion, while the contribution from the remaining panels is computed directly using the underlying Gauss-Legendre quadrature.

Let the boundary be composed of a set of panels  $\Gamma_i$ ,

$$(77) \quad \partial\Omega = \bigcup_i \Gamma_i.$$

We can then denote by  $\mathcal{N}$  the near panels that are included in the local expansion, and by  $\mathcal{F}$  the far panels that are evaluated directly. If we write the layer potential as

$$(78) \quad u^{\partial\Omega}(z) = \int_{\partial\Omega} G(z, w) \sigma(w) ds_w,$$

then the numerical approximation of  $u$  using local QBX can be written as

$$(79) \quad \tilde{u}^{\partial\Omega}(z) = u_{\text{QBX}}^{\mathcal{N}}(z) + u_{\text{direct}}^{\mathcal{F}}(z).$$

To combine this with a fast method that directly evaluates the interactions between all source points (such as the FMM), one can simply subtract the direct contribution from the near panels,

$$(80) \quad \tilde{u}^{\partial\Omega}(z) = u_{\text{fast}}^{\partial\Omega}(z) - u_{\text{direct}}^{\mathcal{N}}(z) + u_{\text{QBX}}^{\mathcal{N}}(z).$$

The last two terms in this expression can together be viewed as a correction term to the direct quadrature. Since this correction only has local support, the local QBX scheme is FMM compatible, in the sense introduced in [11]. This “black box” way of using the fast method could potentially introduce cancellation errors, when the direct contribution from the near panels is added and subtracted, though we have not observed any such problems in practice. The alternative is to modify the FMM to ignore those local contributions in the first place, which is non-trivial for complex geometries.

A subtle feature of local QBX is that the width of the segment  $\mathcal{N}$  affects the convergence rate of the local expansion. This is due to artificially induced endpoint singularities at the interfaces between  $\mathcal{N}$  and  $\mathcal{F}$ , and has been discussed to some extent in both [5] and [19]. The choice of width of  $\mathcal{N}$  is therefore a balance; widening  $\mathcal{N}$  means more points contributing to each expansion, while narrowing  $\mathcal{N}$  gives a slower convergence of the expansion. Actually, not only is the convergence slower, the exponential convergence of the truncation error (14) also tends to be less regular. This in turn makes it harder for AQBX to correctly determine when to terminate. We have found that a good balance is struck by using the five panels that are closest to the expansion center.

**5. Numerical experiments.** We have implemented the above algorithms in Matlab, and used the FMM as implemented in FMMLIB2D [8] for fast far-field evaluations. Timings will not be reported here, as our code is a proof of concept rather than a production implementation. We will in the following numerical experiments only report on the Helmholtz problem, as that is the more challenging one. Carrying out the same experiments for the Laplace problem just results in similar, though slightly better, results.

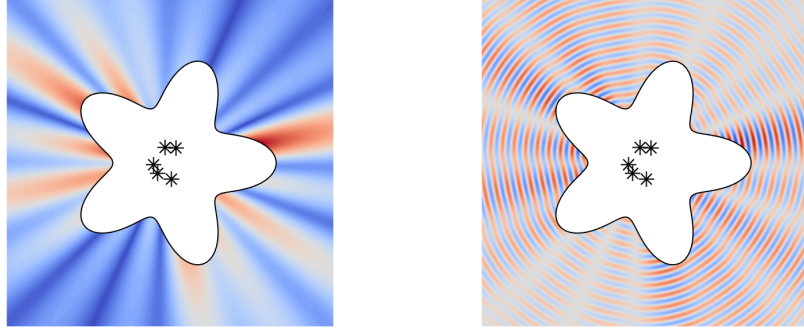


FIG. 5. *Solution to Helmholtz equation given by five point sources located inside a starfish domain. To the left is  $|u(z)|$ , to the right is  $\text{Re } u(z)$ .*

For our experiments we set up the reference problem shown in Figure 5: The Helmholtz problem in the domain exterior to the starfish curve  $\gamma(t) = (1 + 0.3 \cos(10\pi t))e^{2\pi it}$ ,  $t \in [0, 2\pi]$ , with Dirichlet boundary conditions given by the potential from five point sources in the interior domain. We discretize the boundary using 100 Gauss-Legendre panels of order 16 and equal arclength  $h$ , and choose our wavenumber such that  $k = 4/h$ . We position one expansion center at a distance  $r$  in the normal direction from each point on the boundary, and use as a default value  $r = h/4$ . The density  $\sigma$  is computed by solving the integral equation (35) using the Nyström method of [12]. We can then evaluate the layer potential using AQBX, and compare the result to the exact solution given by the potential from the five point sources. The error in AQBX has in our tests always been largest when evaluating the layer potential on the boundary (where the integral is singular), so we mainly report



the errors as measured there. Figure 6 shows the error along the entire boundary when evaluating using AQBX, and also illustrates how the algorithm works. One can clearly see how the magnitude of the coefficients  $a_m$  provides a good overestimate of the truncation error, while the coefficient error is closely tracked by the estimate  $E_C$ . Figure 7 shows example results from when AQBX is

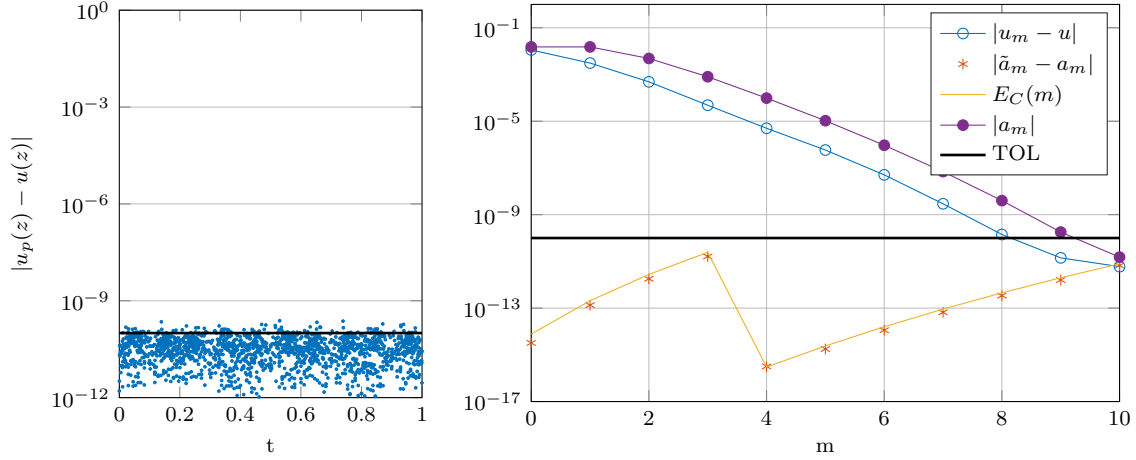


FIG. 6. Results when evaluating the solution to Helmholtz equation using AQBX with tolerance set to  $10^{-10}$ , marked as thick black line. Left: Distribution of error along  $\partial\Omega$ , which shows that the error stays close to the tolerance, though it is not strictly met. Right: Example showing the behavior of AQBX at a single expansion center, when evaluating at the closest boundary point. The error decays exponentially with expansion order, at the same rate as the coefficients  $a_m$ . At the same time the coefficient error  $|a_m - \tilde{a}_m|$  is growing, but is well estimated by the estimate  $E_C(m)$  (73). Note the jump in coefficient error between  $m = 3$  and  $m = 4$ , where the grid is upsampled to maintain the error below tolerance.

used for evaluating the potential in the domain, where the integral is nearly singular. It can be seen that AQBX is only activated at the points where it is needed, and that the potential is then evaluated to the desired accuracy at those points.

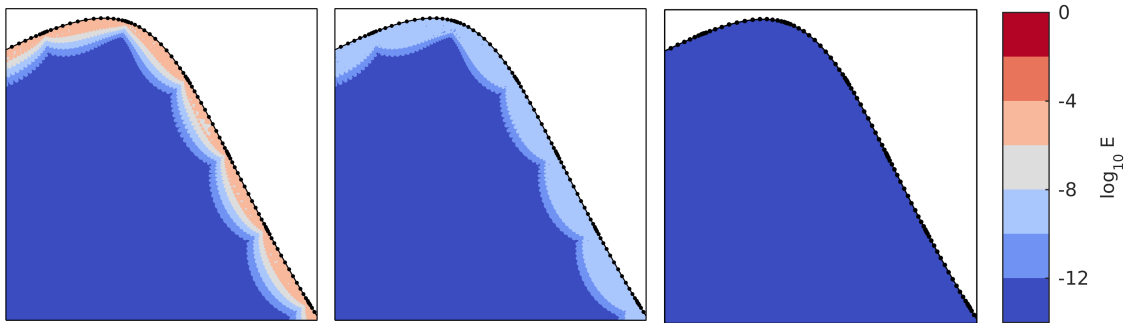


FIG. 7. Errors when evaluating the potential of Figure 5, in the region highlighted in Figure 4. The AQBX tolerance is set to  $10^{-4}$ ,  $10^{-6}$  and  $10^{-12}$ , from left to right, and the region where AQBX is activated is determined using the error estimate for the potential (76).

We believe that the main benefit of using AQBX rather than a direct QBX implementation is that the parameter choice is greatly simplified; given an expansion distance  $r$  and a tolerance  $\epsilon$ , the upsampling rate  $\kappa$  and expansion order  $p$  are set on the fly as needed at each expansion center. A second benefit is that setting  $\kappa$  and  $p$  on the fly can save some work, compared to using fixed values everywhere. In an attempt to quantify this, we now introduce a measure of the work ( $W$ ) needed to form a local expansion, in terms of source evaluations per original source point. If direct QBX is used with order  $p$  and a fixed upsampling rate  $\kappa$ , then the work is given by

$$(81) \quad W_{\text{QBX}} = p\kappa.$$

If AQBX is used to compute  $p$  coefficients, with upsampling rate  $\kappa_m$  used to evaluate the  $m$ th coefficient, then the work is given by

$$(82) \quad W_{\text{AQBX}} = \sum_{m=1}^p \kappa_m.$$

As a comparison, in Tables 1 and 2 we measure the work when computing all expansion coefficients in our reference problem using AQBX, and compare that to the work needed if  $p$  and  $\kappa$  are fixed everywhere to the minimum values required to achieve the same accuracy as AQBX. These fixed values are tuned by hand to the optimal values for this specific problems, yet our algorithm gives a slight speedup in our definition of work. More importantly, our algorithm is in most cases able to keep the error at the desired order of magnitude without any manual intervention, while hand-tuning parameters is strictly unfeasible in real applications.

Our measure of work does not take into account the extra effort needed to evaluate the estimate of the AQBX scheme. The reported speedup should therefore be viewed as an upper limit, and as an indicator that automatic parameter selection does not necessarily have to be more expensive than using fixed parameters set to optimal values. To minimize the overhead of the scheme one can evaluate the error estimates (54) and (74) recursively, and the multiple levels of upsampling can for each panel be computed and reused as needed using a caching algorithm.

| Tol.<br>$\epsilon$ | Eval. error<br>$\ u_p - u\ _\infty$ | Exp. order $p$<br>avg (opt) | Upsamp. rate $\kappa$<br>avg (opt) | Work $W$<br>avg (opt) | Speedup (avg)<br>$W_{\text{AQBX}}/W_{\text{QBX}}$ |
|--------------------|-------------------------------------|-----------------------------|------------------------------------|-----------------------|---|
| $10^{-4}$          | $1.4 \cdot 10^{-3}$                 | 5.4 ( 3)                    | 1.0 ( 2)                           | 5.5 ( 6)              | 1.0   |
| $10^{-6}$          | $2.0 \cdot 10^{-6}$                 | 7.5 ( 5)                    | 1.4 ( 2)                           | 10.2 ( 10)            | 1.0   |
| $10^{-8}$          | $1.9 \cdot 10^{-8}$                 | 9.2 ( 7)                    | 1.8 ( 3)                           | 16.5 ( 21)            | 1.3   |
| $10^{-10}$         | $2.4 \cdot 10^{-10}$                | 10.9 ( 9)                   | 2.2 ( 3)                           | 24.0 ( 27)            | 1.1   |
| $10^{-12}$         | $3.7 \cdot 10^{-12}$                | 12.7 ( 11)                  | 2.5 ( 4)                           | 32.3 ( 44)            | 1.4   |

TABLE 1

*Results for varying tolerance and  $r/h = 1/4$ , comparing AQBX and direct QBX on our reference problem. Error is measured on  $\partial\Omega$ . Reported parameters are for AQBX an average over all expansion centers (avg), and for direct QBX the optimal fixed values used at all centers (opt).*

**6. Conclusions.** We have in this paper formulated a scheme for adaptive quadrature by expansion (AQBX), which allows for the evaluation of singular and nearly singular layer potential integrals on a curve discretized using composite Gauss-Legendre quadrature. The scheme automatically sets parameters in order to satisfy a given tolerance. This is a great simplification compared

| Dist.<br>$r/h$ | Eval. error<br>$\ u_p - u\ _\infty$ | Exp. order $p$<br>avg (opt) | Upsamp. rate $\kappa$<br>avg (opt) | Work $W$<br>avg (opt) | Speedup (avg)<br>$W_{\text{AQBX}}/W_{\text{QBX}}$ |
|----------------|-------------------------------------|-----------------------------|------------------------------------|-----------------------|---|
| 0.10           | $1.5 \cdot 10^{-10}$                | 8.7 ( 7)                    | 3.9 ( 6)                           | 34.4 ( 42)            | 1.2   |
| 0.25           | $2.4 \cdot 10^{-10}$                | 10.9 ( 9)                   | 2.2 ( 3)                           | 24.0 ( 27)            | 1.1   |
| 0.50           | $3.9 \cdot 10^{-10}$                | 14.0 ( 14)                  | 1.6 ( 2)                           | 22.3 ( 38)            | 1.3   |
| 0.75           | $3.4 \cdot 10^{-10}$                | 17.5 ( 21)                  | 1.5 ( 2)                           | 26.9 ( 42)            | 1.6   |
| 1.00           | $1.3 \cdot 10^{-9}$                 | 22.4 ( 39)                  | 1.9 ( 2)                           | 43.2 ( 78)            | 1.8   |

TABLE 2

Results for varying  $r/h$  and tolerance  $\epsilon = 10^{-10}$ , computed in the same way as in Table 1.

to the original QBX scheme, which has a very large parameter space. Given a target tolerance, the only free parameter is here the expansion radius  $r$ . Since the remaining parameters are set on the fly, varying  $r$  will mainly affect the speed of the algorithm. The optimal value for  $r$  with respect to speed will be implementation-dependent, though values of  $W$  in Table 2 suggest that  $r/h$  in the range 1/4–1/2 is a good choice.

The key component of our scheme is the ability to accurately estimate the magnitude of the quadrature errors in the QBX coefficients. To do this we have built on the results of [2], where such estimates were reported for a flat panel. We have extended these to curved panels by taking into account the mapping between a flat panel and a curved panel. This mapping can be locally constructed using only the locations of the quadrature nodes on each panel, and therefore requires no additional analytical information. A side benefit of our estimates is that the nearly singular quadrature error of the underlying layer potential can be accurately estimated, which provides an excellent criterion for when to activate special quadrature also when other methods are used [14, 4]. This could also prove useful for QBX schemes where the expansion is formed by multiple layer potential evaluations in a neighborhood of the expansion center [3, 21].

The focus on a target accuracy is, in our experience, uncommon in the context of singular and nearly singular quadrature. We do however believe that this is important if integral equation methods are to be used in large-scale simulations, where the focus is on achieving a target accuracy at the lowest possible computational cost.

While several excellent special quadrature methods exist in two dimensions, methods in three dimensions have not yet reached the same maturity. The QBX method has been successfully used on simple geometries in 3D [1], while development for more general use is ongoing. If accurate parameter selection is important in 2D, it is absolutely essential in 3D, as costs are higher and the impact of suboptimal parameter choices more severe. The principles of the present 2D scheme can be extended to three dimensions. Estimates for the coefficient errors in 3D were in [2] developed for the special case of spheroidal surfaces. Developing estimates for general surfaces in 3D is a topic of ongoing work, and results will be reported at a later date.

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